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Efficient Use of Prior Information to Calibrate the Gridded Surface Subsurface Hydrologic Analysis (GSSHA) Hydrology Model

by Brian E. Skahill and Charles W. Downer

PURPOSE: The purpose of this document is to provide guidance on the use of two computer-based calibration functionalities recently developed for the Gridded Surface Subsurface Hydrologic Analysis (GSSHA) model. These new capabilities enable the incorporation of *soft* data, or prior information (i.e., extra observations which pertain directly to the estimable parameters, primarily in attempts to stabilize the calibration process). These new calibration methods are not only efficient (measured in terms of forward-model, call-run requirements) but also effective in that they result in physically acceptable models usable for subsequent prediction. This document describes how to use these new functionalities to calibrate a GSSHA model as well as benefits that can be derived in the process.

INTRODUCTION: Spatially explicit, physics-based models such as GSSHA (Downer and Ogden 2003a,b) support a more realistic characterization of the physical aspects of watersheds and a more transparent simulation and evaluation of project alternatives than is possible with traditional hydrologic simulation models (viz., lumped and semidistributed model structures). Such models have the potential to predict with greater reliability than lumped hydrologic model structures (Moore and Doherty 2005). However, they also have the potential to easily become highly parameterized, particularly when deployed to simulate a heterogeneous watershed on a continuous basis. Simulation times with such models are often far greater than with lumped and semidistributed hydrologic models.

It is this combination of computationally intensive, forward model run times and the potential for a highly dimensional, specified adjustable model parameter space which presents a unique challenge for the computer-based calibration of spatially explicit, physics-based hydrologic models. In particular, this combination necessitates the use of a calibration method that is as efficient as possible. Hydrologic models are typically calibrated by adjusting parameters encapsulated in the simulator until there is an acceptable level of agreement between a set of historical data and their model simulated counterparts. Highly parameterized model deployments (10s to 100s of parameters) can also make calibration problematic in that the information content of the available observed data may not support the unique estimation for each of the specified adjustable model parameters, resulting in a poor calibration and/or non-physical models. Efficient calibration methods are needed that result in believable models which yield acceptable fits with the observed dataset, particularly for challenging model calibration situations.

This document describes how to use two separate, but closely related, methods of computer-based parameter estimation either can serve as an effective and efficient means to support the practical

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calibration of a GSSHA hydrologic model. The two methods are adaptations to the “efficient local search” calibration methodology (Skahill and Downer 2012.)

The two model calibration methods described herein are both highly efficient, much in the same way as the “efficient local search” method is as described in Skahill and Downer (2012), Skahill et al. (2012), and Skahill et al. (2009). Both approaches tackle the problem of calibration parameter insensitivity by incorporating additional data (which pertains directly to the specified adjustable model parameters) into the parameter-estimation process. These extra observations effectively stabilize the model calibration process and are often referred to as prior information or regularization constraints. With each of these two methods, parameters that cannot be uniquely estimated are provided with values, or assigned relationships with other parameters, that are determined to be realistic by the modeler. The examples profiled in the following demonstrate two concrete and unique specifications of prior information or regularization relationships in attempts to make them better understood to the reader.

Conversely, where the calibration dataset is able to support estimates to be made of the values of many parameters, the making of such estimates is not precluded by pre-emptively reducing the dimensionality of estimable parameter space ahead of the calibration process. During hydrologic model development, watershed system detail is reflected either because it is presumed to be of relevance or is in fact identified a priori as necessary for the predetermined, alternative-scenario predictions of interest. However, this desired and/or required model complexity is often not supported by either the quantity and/or the type of observed system-state data that is available for model calibration. This noted potential mismatch in reflected model detail relative to the information available in the observed data may make calibration problematical, particularly for a highly parameterizable hydrologic model. In this situation, the calibration process may become numerically unstable by virtue of parameter insensitivity and/or parameter correlation, resulting in less than, if not far from, optimal fits to the data, and associated nonphysical parameter sets. The two methods described in this technical note complement a potentially highly parameterizable hydrologic model by allowing one to incorporate outside information (viz., prior information) into the calibration process.

The first of the two methods to be described is the secant Levenberg-Marquardt (SLM) method, the basis for the “efficient local search” alternate GSSHA run mode, adapted to support prior information. The second method is the SLM version of the Tikhonov solution (Greenhalgh et al. 2006). As previously mentioned, this technical note describes the practical use of these two methods to calibrate a GSSHA model. The active reader is directed to Greenhalgh et al. (2006) and references cited therein for mathematical and theoretical details underpinning the two related calibration methods.

DESCRIPTION OF USE: In describing how to use these two methods, it is assumed that the files necessary to calibrate a GSSHA model with the “efficient local search” method using the previously mentioned available guidance have already been prepared. Only the additional steps necessary to use the two methods will be described. For each of the two methods, the [example problem](#) prepared as part of Skahill and Downer (2012) will be the starting point of the two example problems. In each case, a step-by-step description of the modifications required to use either method will be described. For each of the methods, the two examples will present two different approaches to consider for specifying prior information or regularization relationships.

The model to be calibrated was designed for the purposes of testing, evaluating, and demonstrating new GSSHA model calibration methods. Briefly, it is a 200 meter grid cell scale single event (06/30/2009–07/02/2009) simulation model of the approximately 20 square mile Goodwin Creek Experimental Watershed (GCEW) (Downer and Ogden (2003b) and references cited therein for details regarding the GCEW dataset). Eight GSSHA model parameters were specified as adjustable (viz., three overland flow roughness and five soil vertical hydraulic conductivity values for the three land use and five soil types which, respectively, constitute the GCEW land area for the GSSHA model as it was developed). Simulated flows at the watershed outlet, transformed using a Box-Cox transformation (Box and Jenkins 1976), and synthetically generated with a known parameter set, constituted the observed dataset for model calibration.

Method 1: Secant Levenberg Marquardt method with prior information:

Example 1

This example employs the “efficient local search” method adapted to include prior information. The prior information is specified to effect a preferred homogeneity condition (viz., that all adjustable model parameters of the same type are specified to be the same value). In particular, for the GSSHA model to be calibrated, all three overland roughness values and all five soil vertical hydraulic conductivity values are specified to be the same, respectively. This approach with prior information effectively reduces the dimensionality of the problem in that specified adjustable model parameters of the same type are now enforced to be the same value during model calibration. The model problem is now being biased to be more spatially grouped with respect to parameterization. The degree to which the prior information is in fact enforced is dependent upon their weights assignment and also the information content of the observation dataset to support the unique estimation for the adjustable parameters. This regularization strategy certainly may be justified, particularly if it is employed for the simultaneous calibration of multiple adjacent subwatershed models where it can effectively be argued that hydrologic response is similar across the modeled systems. The files for this example problem are available for download and use from http://www.gsshawiki.com/images/e/e8/Example1_PI.zip.

1. Copy the contents of the [example](#) problem to a new and empty directory on your local hard drive.
2. Make a copy of the control file named “cal_003.pst” and name the copy “cal_003_pi.pst”.
3. Add the nine lines, that follow, to the end of the control file named “cal_003_pi.pst”. In so doing, eight individual pieces of prior information for the eight specified adjustable model parameters now enforce the previously mentioned preferred homogeneity condition. As indicated previously (Skahill and Downer 2012; Skahill et al. 2012; Skahill et al. 2009), the computer-based calibration methods are written to accommodate a popular input-file protocol (Doherty 2004), and this also applies for the specification of prior information. The log of each adjustable model parameter is used in each prior information equation since each parameter is log transformed as indicated in the second entry on each of the eight rows which constitute the “parameter data” section of the control file. The eight pieces of prior information are uniformly weighted with a value of 1, and each of their individual contributions are aggregated into a single new observation group named “pinfo”, which will be added in the next step to the global quantitative measure of model-to-measurement misfit.

* prior information

pi1 1.0 * log(rough1) - 1.0 * log(rough2) = 0.0 1 pinfo

pi2 1.0 * log(rough2) - 1.0 * log(rough3) = 0.0 1 pinfo

pi3 1.0 * log(rough3) - 1.0 * log(rough1) = 0.0 1 pinfo

pi4 1.0 * log(ksat1) - 1.0 * log(ksat2) = 0.0 1 pinfo

pi5 1.0 * log(ksat2) - 1.0 * log(ksat3) = 0.0 1 pinfo

pi6 1.0 * log(ksat3) - 1.0 * log(ksat4) = 0.0 1 pinfo

pi7 1.0 * log(ksat4) - 1.0 * log(ksat5) = 0.0 1 pinfo

pi8 1.0 * log(ksat5) - 1.0 * log(ksat1) = 0.0 1 pinfo

4. Modify the “observation groups” section of the control file to now also include the single prior information observation group named “pinfo” on a new line after the observation group named “tmfl”.
5. Modify the second line of the control data section of the control file to indicate that there are now **8** pieces of prior information and **2** observation groups as indicated here:

* control data

restart estimation

8 97 8 **8 2**

6. Save the control file.
7. Run (calibrate) the GSSHA model by opening up a command window, typing the following at the prompt, and pressing enter:

gssha -slm cal_003_pi.pst

The computer-based GSSHA model calibration run for this example problem reduced the global quantitative measure of model-to-measurement misfit from an original value of approximately 34.84 to a final value of 0.03347 upon the completion of five optimization iterations (the maximum number of optimization iterations to be performed as specified in the control data section of the control file (it is typically set to be around 30)), which equated to 28 forward GSSHA model calls. The final estimated values for the eight specified adjustable model parameters ((rough1, rough2, rough3, ksat1, ksat2, ksat3, ksat4, ksat5) = (0.100364, 0.095635, 0.096860, 0.105406, 0.132966, 0.144165, 0.150000, 0.113480)) and their computed confidence limits are listed in the record file named “cal_003_pi.rec”.

The final estimated parameter values for the computer-based GSSHA model calibration run that are listed in Table 1 underscore that the weights-assignment strategy for the prior information did in fact enforce the specified preferred parameter state. The adjustable model parameter named “ksat4” hit its lower bound as the method attempted to simultaneously enforce the model fit to the observed data and the prior information conditions. The variation observed in Table 1 amongst the

values for parameters of the same type suggests that the information content of the observed dataset did support a deviation from exact enforcement of the specified prior information equations. The active reader is encouraged to explore different weights assignments for the prior information (and the observed data) in this example problem to learn how it impacts fit to the observed data and also fit to the specified prior information.

Table 1. Estimated parameter values resulting from the "SLM with prior information" GSSHA model calibration run.

Parameter	rough1	rough2	rough3	ksat1	ksat2	ksat3	ksat4	ksat5
Estimated Value	0.104	0.096	0.097	0.105	0.133	0.144	0.150	0.113

The same model was also calibrated using the original control file named "cal_003.pst" by typing "gssha -slm cal_003.pst" at the command prompt and pressing enter. The final estimated model for this GSSHA model calibration run without any use of prior information is (rough1, rough2, rough3, ksat1, ksat2, ksat3, ksat4, ksat5) = (0.091778, 0.096802, 0.491869, 0.084113, 0.287828, 1.211571, 0.336561, 2.758958). During execution of the model calibration run with the original control file named "cal_003.pst", four of the eight specified adjustable model parameters were indicated to have no effect on observations (viz., "rough3", "ksat3", "ksat4", and "ksat5"). Clearly, the GSSHA model calibration problem encapsulated in the original control file named "cal_003.pst" was in fact a good candidate for stabilization via the specification of prior information or regularization relationships.

Example 2

This example also employs the "efficient local search" method adapted to include prior information. The prior information equations in this example define explicit preferred parameter values (viz., (rough1, rough2, rough3, ksat1, ksat2, ksat3, ksat4, ksat5) = (0.2, 0.3, 0.4, 0.1, 0.5, 1.5, 0.3, 0.2)). The files for this example problem are available for download and use from http://www.gsshawiki.com/images/6/62/Example2_PI.zip.

1. Copy the contents of the [example](#) problem to a new and empty directory on your local hard drive.
2. Make a copy of the control file named "cal_003.pst" and name the copy "cal_003_pi2.pst".
3. Add the nine lines, that follow, to the end of the control file named "cal_003_pi2.pst". In so doing, eight individual pieces of prior information for the eight specified adjustable model parameters now enforce the previously mentioned preferred parameter values. As with Example 1, the log of each adjustable model parameter is used in each prior information equation since each parameter is log transformed as indicated in the second entry on each of the eight rows which constitute the "parameter data" section of the control file. The eight pieces of prior information are uniformly weighted with a value of 1, and each of their individual contributions to now be added to the global quantitative measure of model-to-measurement misfit are aggregated into a single new observation group named "pinfo":

* prior information

pi1 1.0 * log(rough1) = -0.69897000 1 pinfo

pi2 1.0 * log(rough2) = -0.52287875 1 pinfo

pi3 1.0 * log(rough3) = -0.39794001 1 pinfo

pi4 1.0 * log(ksat1) = -1.00000000 1 pinfo

pi5 1.0 * log(ksat2) = -0.30103000 1 pinfo

pi6 1.0 * log(ksat3) = 0.176091260 1 pinfo

pi7 1.0 * log(ksat4) = -0.52287875 1 pinfo

pi8 1.0 * log(ksat5) = -0.69897000 1 pinfo

4. Modify the “observation groups” section of the control file to now also include the single prior information observation group named “pinfo” on a new line after the observation group named “tmf1”.
5. Modify the second line of the control data section of the control file to indicate that there are now **8** pieces of prior information and **2** observation groups as indicated here:

* control data

restart estimation

8 97 8 **8 2**

6. Save the control file.
7. Run (calibrate) the GSSHA model by opening up a command window, typing the following at the prompt, and pressing enter:

gssha -slm cal_003_pi2.pst

The computer-based GSSHA model calibration run for this example problem reduced the global quantitative measure of model-to-measurement misfit from an original value of approximately 32.86 to a final value of 0.4123 upon the completion of five optimization iterations (the maximum number of optimization iterations to be performed as specified in the control data section of the control file), which equated to 24 forward GSSHA model calls. The final estimated values for the eight specified adjustable model parameters are listed in Table 2. The weight assigned to each piece of prior information in this example was 1, just as with the first example. Clearly, the same weighting strategy more easily enforced the prior information that was specified with the first example. Of course, stronger enforcement of the prior information via a different weights assignment strategy would yield a final estimated model most likely in closer agreement with the preferred model specified in the prior information, but possibly at a cost with respect to fit to the observed data.

Table 2. Estimated parameter values resulting from the "SLM with prior information" GSSHA model calibration run.

Parameter	rough1	rough2	rough3	ksat1	ksat2	ksat3	ksat4	ksat5
Estimated Value	0.092	0.287	0.418	0.071	0.505	1.432	0.308	0.355

Method 2: Secant Levenberg Marquardt version of the Tikhonov solution:

This method differs from the first in that it has a regularization weight multiplier (β^2) which permits the modeler to explicitly explore the tradeoff between fit to the observed data and fit to the regularization relationships. Just as with the first method with prior information, the regularization relationships are weighted; however, with this approach, they are subsequently multiplied by a regularization weight factor (β^2). Selection of an appropriate value for β^2 is critical. If the β^2 value is too high, the parameter estimation process will ignore the measurement dataset in favor of fitting the regularization observations. If the β^2 value is too small, the regularization observations will not endow the parameter estimation process with the numerical stability which it needs in order to obtain estimates for the parameters. In this way, the assignment of a value to β^2 can be viewed as a mechanism for trading parameter reasonableness against goodness of fit. There are several means by which to estimate an optimal fixed value for β^2 , but in the two examples below, there will be demonstrated one approach (Hansen 2001). The files for this example problem are available for download and use from http://www.gsshawiki.com/images/1/19/Example1_Tik.zip.

Example 1

This is the same Example 1 calibration problem previously considered with the first method.

1. Copy the contents of the [example](#) problem to a new and empty directory on your local hard drive.
2. Make a copy of the control file named "cal_003.pst" and name the copy "cal_003_tik_001.pst".
3. Add the prior information to the control file in exactly the same way as it was added in Step 3 of Example 1 with the first method.
4. Modify the observation-groups section of the control file in the same way as it was in Step 4 of Example 1 with the first method.
5. Modify the second line of the control data section of the control file in the same way as was done in Step 5 of Example 1 with the first method.
6. On the first line of the control data section, change "estimation" to "regularization" to activate use of the second method.
7. Not only to activate the implementation of the Tikhonov solution, which differs from that of Doherty (2004) but also to remain consistent with his input file protocol, add the four lines, that follow, to the end of the control file. The only input of importance below being specification of the regularization weight factor which in this case is specified to be 1.

* regularisation

10.0 11.0 0.0

1.0e0 1.0e0 1.0000000001e0

1.3 1.0e-2 0

8. While it is not necessary, in this case for this method, in attempts to focus on the influence of the regularization relationships, during testing the de-facto stabilization device that is a part of both methods was effectively set to zero (1E-14). It is recommended that for typical applications this algorithm input setting be operative and to be specified with a default value of 5.0. In addition, the input control setting which specifies the maximum number of parameter upgrades to be tested at each optimization iteration was set to 1 given that the de-facto stabilization device was deactivated. This input setting is typically specified with a value of 10. These two changes are made on the fourth line of the control data section of the control file as indicated here in bold:

0.000000000000001 2.0 0.3 0.03 **1**

9. Of course, in practice, the initial parameter values that are specified should reflect the best information available to support their estimation. And moreover, their specified bounds should be consistent with the employed model parameterization scheme. In this model calibration problem, the specified regularization relationships are to enforce a homogeneity condition across like parameters. For simplicity and for the purposes of illustrating the methodology with little complication, there is a slight departure from regular calibration practice. While it is also not necessary, the parameter data section of the control file (Doherty 2004) is also modified such that (a) the initial parameter set is 0.1, and (b) the lower and upper bounds for each of the two parameter types are uniformly the same, as indicated in the fourth and also the fifth and sixth columns, respectively:

* parameter data

rough1	log factor	0.1	1.00000E-02	5.00000E-01	rough1	1.000	0.000	1
rough2	log factor	0.1	1.00000E-02	5.00000E-01	rough2	1.000	0.000	1
rough3	log factor	0.1	1.00000E-02	5.00000E-01	rough3	1.000	0.000	1
ksat1	log factor	0.1	6.60000E-03	2.99	ksat1	1.000	0.000	1
ksat2	log factor	0.1	6.60000E-03	2.99	ksat2	1.000	0.000	1
ksat3	log factor	0.1	6.60000E-03	2.99	ksat3	1.000	0.000	1
ksat4	log factor	0.1	6.60000E-03	2.99	ksat4	1.000	0.000	1
ksat5	log factor	0.1	6.60000E-03	2.99	ksat5	1.000	0.000	1

10. Save the control file.

11. Run (calibrate) the GSSHA model by opening up a command window, typing the following at the prompt, and pressing enter:

```
gssha -slm cal_003_tik_001.pst
```

The GSSHA model was also calibrated with this second method five additional times with five separate and unique values for the regularization weight factor (viz., 0.01, 0.1, 0.5, 0.75, 1.0 and 10). Figure 1 presents the final estimated values which quantified model-to-measurement misfit with respect to the observations and also the regularization relationships for each of the six GSSHA model-calibration runs. The plot clearly indicates the previously mentioned explicit tradeoff associated with varying the value for the regularization weight factor. Because the measurement/regularization objective function is an increasing/decreasing function of β^2 , a plot of their optimal values often takes on the shape of an “L”. A popular means by which to select an optimal value for β^2 is to select that solution which is closest to the corner of the L (Hansen 2001). The L-curve criterion would suggest that an optimal value to select for β^2 to calibrate this problem as otherwise designed is approximately 0.75.

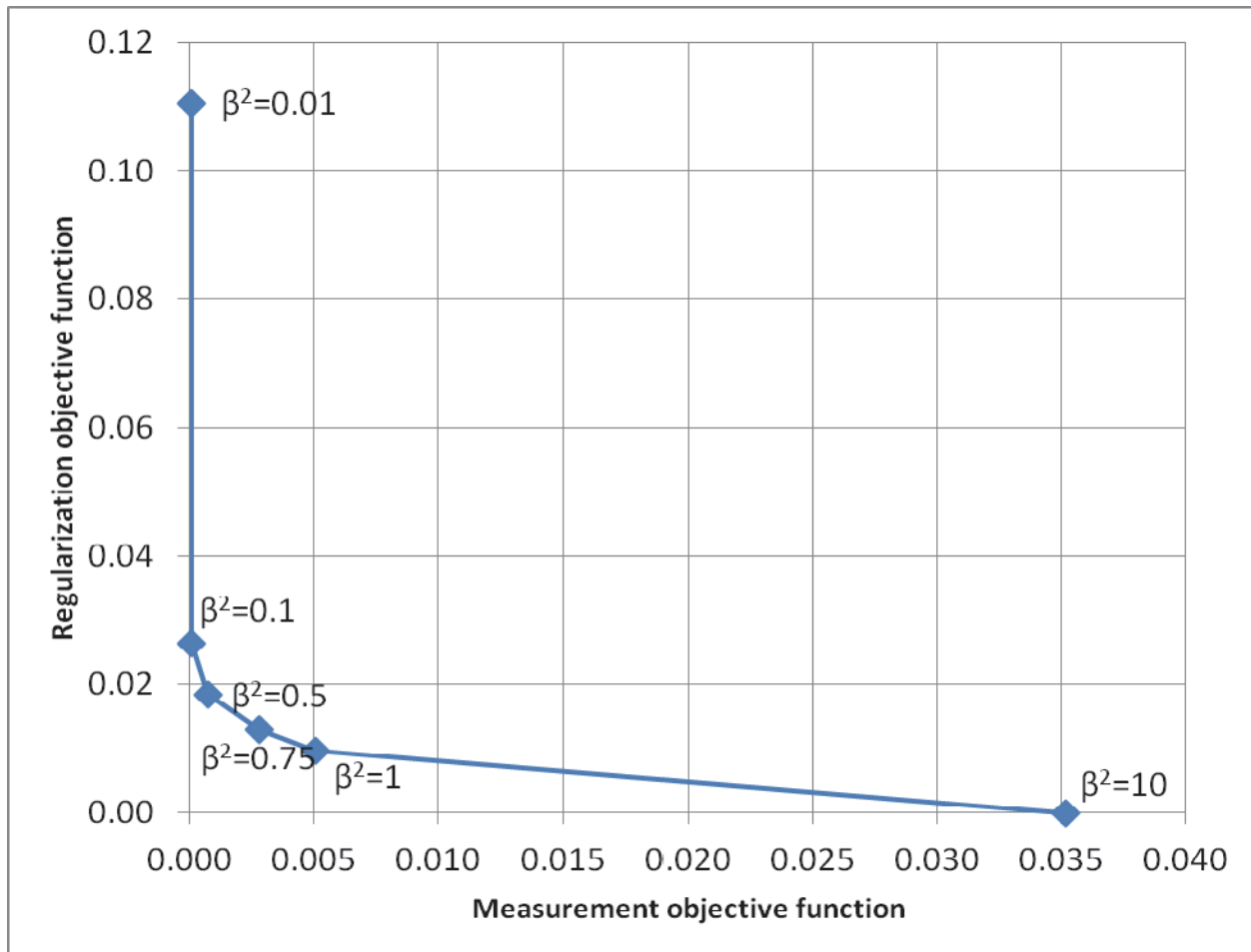


Figure 1. L-curve for Method 2, Example 1.

Example 2

This is the same Example 2 calibration problem previously considered with the first method. The files for this example problem are available for download and use from http://www.gsshawiki.com/images/5/59/Example2_Tik.zip.

1. Copy the contents of the [example](#) problem to a new and empty directory on your local hard drive.
2. Make a copy of the previously prepared control file named “cal_003_tik_001.pst”, name the copy “cal_003_tik_101.pst”, and place this file in the new directory created in the previous step.
3. Change the seventh line of the control data section of the control file to be the following, which modifies the termination criteria for the method:

```
30 .001 4 4 .001 4
```

4. Change the parameter data section of the control file to the following:

```
* parameter data
```

```
rough1 log factor 0.4      1.00000E-02 0.50 rough1 1.000 0.000 1
rough2 log factor 0.2      1.00000E-02 0.50 rough2 1.000 0.000 1
rough3 log factor 0.3      1.00000E-02 0.50 rough3 1.000 0.000 1
ksat1  log factor 0.5      1.50000E-02 0.61 ksat1 1.000 0.000 1
ksat2  log factor 0.1      1.50000E-02 0.61 ksat2 1.000 0.000 1
ksat3  log factor 0.1      6.60000E-02 2.99 ksat3 1.000 0.000 1
ksat4  log factor 0.4      1.50000E-01 0.61 ksat4 1.000 0.000 1
ksat5  log factor 0.1      6.60000E-03 2.99 ksat5 1.000 0.000 1
```

5. Change the prior information section to be the same as that specified in item 3 for the second example problem considered with the first method.
6. Save the control file.
7. Run (calibrate) the GSSHA model by opening up a command window, typing the following at the prompt, and pressing enter:

```
gssha -slm cal_003_tik_101.pst
```

8. The GSSHA model was also calibrated with this second method seven additional times for a total of eight separate and unique values for the regularization weight factor (viz., 0.1, 0.25, 0.5, 1.5, 2, 5, and 10). Figure 2 presents the final estimated values which quantified model-to-measurement misfit with respect to the observations and also the regularization relationships for each of the eight GSSHA model calibration runs. Clearly,

the plot indicates the previously mentioned explicit tradeoff associated with varying the value for the regularization weight factor. The L-curve criterion would suggest that an optimal value to select for β^2 to calibrate this problem as otherwise designed is approximately 2 (Hansen 2001).

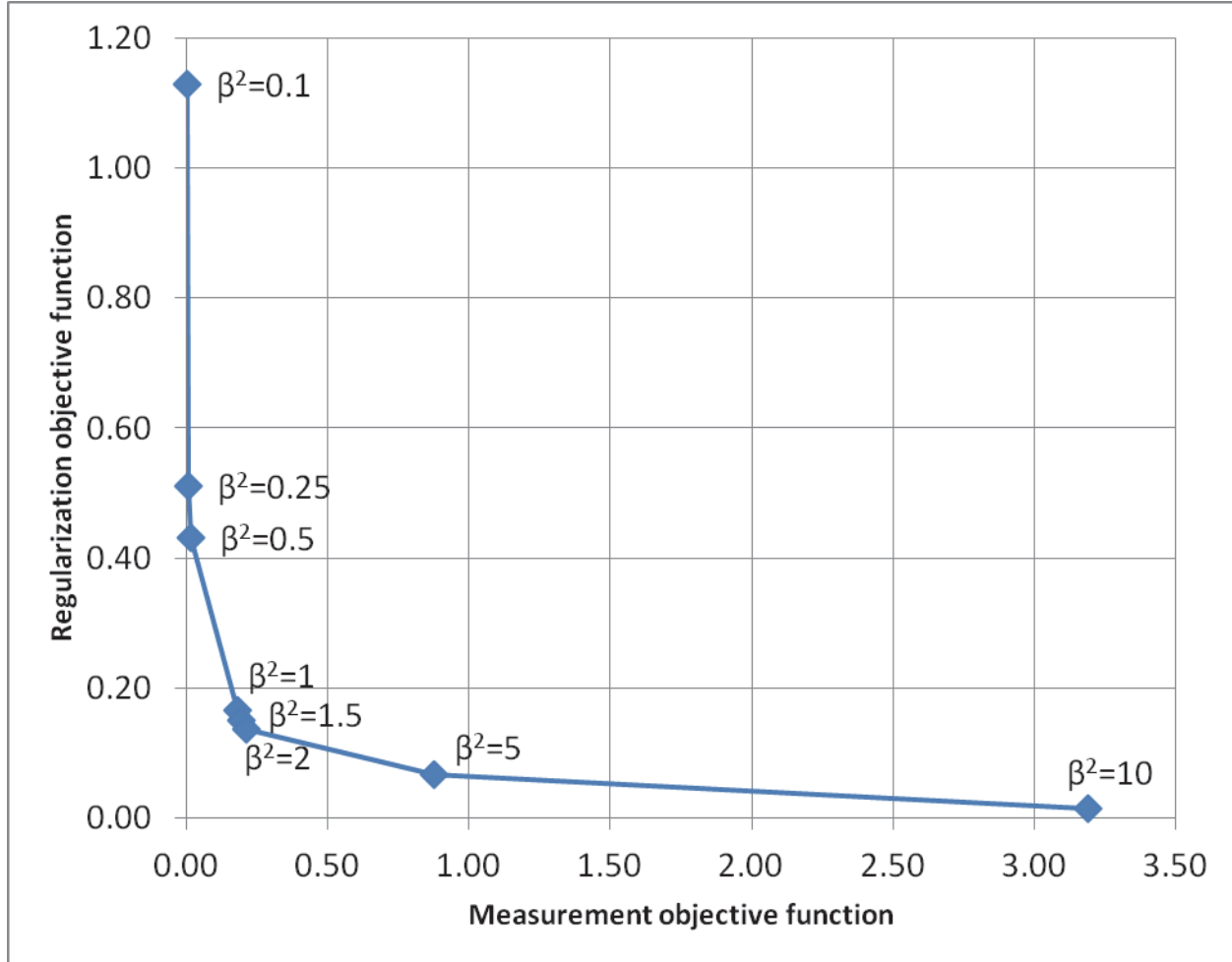


Figure 2. L-curve for Method 2, Example 2.

DISCUSSION AND SUMMARY: This article describes, by way of examples, how to use two, new, closely related methods that can be employed to efficiently calibrate a GSSHA hydrologic model and in that process yield physically acceptable models usable for prediction. They are both adaptations to the previously reported upon “efficient local search” GSSHA model calibration methodology (Skahill and Downer 2012 and references cited therein; http://www.xmswiki.com/xms/WMS:GSSHA_Calibration; http://www.xmswiki.com/xms/WMS:WMS_Tutorials#Distributed_Hydrologic_Modeling_using_GSSHA). The two new methods both achieve calibration-run efficiency in the same way as the “efficient local search” method. Also, they both make what may otherwise be problematical calibration settings effective through the introduction of extra observations which pertain directly to the estimable parameter set. Both approaches are a local search biased toward a specified preferred system state. The degree to which the model is biased is influenced by the prior information weights-assignment strategy, and in the case of the second

method, also the value for the regularization weight multiplier which allows for the explicit evaluation of the tradeoff between fit to the observed data and fit to the regularization relationships.

Efficient methods which permit the specification of regularization constraints hold strong promise as practical means for the calibration of potentially computationally expensive and highly parameterized modeling contexts which can be associated with physics-based, spatially explicit, surface hydrology models, such as GSSHA. For this reason the use of either of these two methods is recommended for the calibration of most practical applications of the GSSHA model. The SLM method with prior information is less complicated to employ; however, the SLM version of the Tikhonov solution includes an explicit parameter for exploring the tradeoffs associated with fits to the observed data and the relationships specified to regularize the solution. The preferred method will depend on available project resources for model calibration and the degree to which the modeling team wishes to explore the noted tradeoff analysis associated with the two calibration methods.

The active reader is encouraged to explore further by experimenting with the example problem datasets. Planned future work will focus on updating the WMS interface to support these two new recommended GSSHA model calibration functionalities.

ADDITIONAL INFORMATION: For additional information, contact Dr. Brian E. Skahill or Dr. Charles W. Downer at Brian.E.Skahill@usace.army.mil and Charles.W.Downer@usace.army.mil, respectively. This CHETN should be cited as follows:

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